

# Shape and blocking effects on odd-even mass differences and rotational motion of nuclei

F.R. Xu,<sup>1,\*</sup> R. Wyss,<sup>2</sup> and P.M. Walker<sup>1</sup>

<sup>1</sup>*Department of Physics, University of Surrey, Guildford, Surrey GU2 5XH, England*

<sup>2</sup>*Department of Physics, Royal Institute of Technology, Frescativägen 24, S-104 05 Stockholm, Sweden*

Nuclear shapes and odd-nucleon blockings strongly influence the odd-even differences of nuclear masses. When such effects are taken into account, the determination of the pairing strength is modified resulting in larger pair gaps. The modified pairing strength leads to an improved self-consistent description of moments of inertia and backbending frequencies, with no additional parameters.

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Since the BCS theory was applied to atomic nuclei [1,2], pairing correlations have been crucial to the understanding of many properties, such as binding energies, collective rotational motion and quasiparticle excitation energies. The interaction strength,  $G$ , of the pairing force is the key parameter that governs the properties of the short range correlations.

The  $G$  value is usually determined by fitting the BCS pairing gaps ( $\Delta = G \sum_i U_i V_i$ ) of even-even nuclei to experimental odd-even mass differences,  $D_{oe}$  (where  $U_i$  and  $V_i$  are the emptiness and occupation amplitudes of nucleon pairs) [2]. However, when one calculates theoretical  $D_{oe}$  values (i.e. in the same manner as calculating experimental  $D_{oe}$  values, but with theoretical nuclear masses) with the  $G$ -value determined according to the above prescription, it turns out that they do not agree with experiment. The theoretical values are systematically smaller than the pairing gaps, at least for the rare-earth deformed nuclei described below. In principle, experimental odd-even mass differences should be compared with theoretical  $D_{oe}$  values. Hence, the pairing strength  $G$  should be adjusted to reproduce, at least on average, theoretical odd-even masses and not pair gaps of even-even nuclei.

Although pairing correlations are dominantly responsible for odd-even mass differences, there exist other non-negligible effects, in view of the systematic differences mentioned above [3]. One important effect stems from the deformed mean field. Due to the Kramers degeneracy of single-particle levels, odd- and even-nucleon systems will have different energies in a deformed field. The interplay between pairing and this ‘mean field’ effect has been clarified in a recent work by Satula *et al.* [4]. For light- and medium-mass nuclei, it is comparable with the pairing contribution [4]. Furthermore, when neighbouring nuclei (which are involved in calculating odd-even mass differences) have different deformations, shape-changing effects will also play a role. These two factors originate from the mean field and we will refer to them in the following as *shape* effects.

Another important influence is the blocking effect. Experimental odd-even mass differences contain the odd-nucleon blocking effect in adjacent odd-particle systems, which is absent in even systems [2,5]. This effect can become significant, especially when the densities of single-particle levels around the neutron and proton Fermi surfaces are not very high. Simple BCS calculations typically show that odd-nucleon blockings reduce pairing gaps by more than 10% for the nuclei in the rare-earth region. Both the shape and blocking effects will influence the determination of the pairing strengths.

Two very sensitive probes of pairing correlations, and therefore of the pairing strengths, are moments of inertia (see e.g. [2,6,7]) and backbending (bandcrossing) frequencies [8,9]. States of high seniority may serve as another probe, and recent calculations of the energies of multi-quasiparticle states show the need for adjustment of the pairing strength [10]. Hence, the question arises as to whether the pairing strength determined from odd-even mass differences is consistent with the pairing strength used to calculate moments of inertia or energies of high seniority states. A consistent way to determine the  $G$ -value is therefore an important issue for the quantitative description of nuclear properties. In this paper, we show that when shape and blocking effects are taking into account, the pairing strength  $G$  needs to be modified in order to reproduce experimental  $D_{oe}$  values. Such modifications result in an improved self-consistent description for both moments of inertia and band-crossing frequencies.

In order to minimize the influences of the quantities that are not relevant for our discussion, we use the five-point formula of Ref. [11] to determine experimental  $D_{oe}$  values. For an even-even nucleus,

$$D_{oe} = -\frac{1}{8}[M(N+2) - 4M(N+1) + 6M(N) - 4M(N-1) + M(N-2)], \quad (1)$$

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\*Permanent address: Department of Technical Physics, Peking University, Beijing 100871, China

where  $M(N)$  is the mass of an atom with neutron number,  $N$  (or  $Z$  for protons). The quantity,  $D_{oe}$ , is calculated along an isotopic (or isotonic) chain. With Eq.(1) we investigate shape and blocking effects using the deformed Woods-Saxon (WS) model [12,13]. According to the Strutinsky energy theorem [14], the total energy of a nucleus can be decomposed into a macroscopic and microscopic part. The latter consists of shell and pairing correction energies. For the macroscopic energy, we employ the standard liquid-drop model of Ref. [15]. Pairing correlations are treated by a technique of approximate particle-number projection, known as the Lipkin-Nogami (LN) method [16] which takes particle-number-fluctuation effects into account by introducing an additional Lagrange multiplier,  $\lambda_2$ . Both monopole and quadrupole pairings are included for residual two-body interactions.

Nuclear shapes are determined by minimizing calculated potential-energy-surface (PES) energies in the quadrupole deformation ( $\beta_2, \gamma$ ) space with hexadecapole ( $\beta_4$ ) variation. For well-deformed nuclei, pairing energies only weakly influence equilibrium deformations [10,14]. Therefore, we use the monopole pairing strengths obtained by the average gap method [11] to determine nuclear deformations. The quadrupole pairing strength is determined by restoring the local Galilean invariance with respect to quadrupole shape oscillations [17,18]. Whereas quadrupole pairing is essential for the proper description of the moments of inertia [19,20], its influence on nuclear binding energies is negligible, since we use the doubly-stretched quadrupole operators [18,21].

In the present work, we focus on well-deformed rare-earth nuclei where an abundance of regular collective rotational bands with backbending have been observed. The shape effects, coming from the shell-correction and the macroscopic deformation energies, can be calculated using Eq.(1), after determining the equilibrium deformations. Our calculations show that the shape effects are usually of the order of 100 to 200 keV for a range of even-even Er, Yb, Hf and W isotopes. If one neglects the changes of deformation, the shape effect for a deformed even system ( $N = 2n$ ) can be written as  $\frac{1}{2}(e_{n+1} - e_n)$  for the three-point formula [4] or  $\frac{1}{4}(e_{n+1} - e_n)$  for the five-point formula of Eq.(1) (where  $e_i$  is the single-particle energy). Shape effects calculated from the above simple forms differ from those calculated according to Eq.(1), when shape changes are included. This implies that the polarization effects of the odd nucleons have to be considered explicitly, as is done in the present work. In contrast to light nuclei [4], the mean-field effects for heavy nuclei are not so large due to the relatively close spacing of the single-particle levels.

In the LN model (for the case of monopole pairing) the quantity,  $\Delta + \lambda_2$ , is assumed to be identified [11] with the odd-even mass difference,  $D_{oe}$ , provided that other physical influences (e.g. shape and blocking effects) are ignored. Hence, the additional contribution coming from the blocking effect can be defined as

$$\delta_{\text{block}} = D_{oe}^{\text{pair}} - (\Delta + \lambda_2) , \quad (2)$$

where the  $D_{oe}^{\text{pair}}$  is the theoretical odd-even difference of pairing energies. The  $D_{oe}^{\text{pair}}$  values are calculated using Eq.(1) with the odd-nucleon blocking effect taken into account. Note that blocking also affects the pairing self energy (Hartree-term), which also contributes to the  $D_{oe}^{\text{pair}}$  value. If the blocking (and deformation changing) effects were neglected, we should have  $D_{oe}^{\text{pair}} \approx \Delta + \lambda_2$ . Since both the  $D_{oe}^{\text{pair}}$  and  $\Delta + \lambda_2$  values increase (decrease) with increasing (decreasing) pairing strengths, the  $\delta_{\text{block}}$  values are not very sensitive to the changes in the  $G$  values. We calculate the blocking effects with the  $G$  values obtained by the average gap method [11]. The results show that the blocking effects are usually about -200 to -400 keV for the rare-earth nuclei. The shape and blocking effects partially cancel, but non-zero effects remain systematically.

The obtained shape and blocking effects,  $\delta$ , are shown in Fig.1. These values range mostly from -100 to -300 keV or about 10% to 30% of the corresponding odd-even mass differences, clearly suggesting that one cannot neglect this component. Note, that the size and the fluctuations of  $\delta$  reflect two different ways to calculate odd-even mass differences, and not the difference between experimental and theoretical odd-even masses.

In general, the shape and blocking effects change smoothly with particle number and one would like to separate the contributions from  $\delta_{\text{shape}}$  and  $\delta_{\text{block}}$ . However, the situation can become rather complex: For  $N = 98\text{--}102$ , the calculated PES's show that the nuclei are soft in  $\beta_2$  deformation, particularly for  $^{172\text{--}176}\text{W}$ . The  $\beta_2$  softness results in relatively large uncertainties in the determination of the  $\beta_2$  values and hence significantly influences the  $\delta_{\text{shape}}$  values. The same holds for the  $\delta_{\text{block}}$  values, leading to fluctuating results. Hence, separate consideration of the  $\delta_{\text{shape}}$  and  $\delta_{\text{block}}$  values can be misleading. In contrast, the combined value of the shape and blocking effects is less shape dependent, since the total energy of a nucleus is not so sensitive to the deformation value in a range around the minimum of a soft PES.

With the above shape and blocking effect ( $\delta$ ) theoretical odd-even mass differences ( $D_{oe}^{\text{th}}$ ) can be determined, and compared with experimental values ( $D_{oe}^{\text{expt}}$ ) to obtain the pairing strengths. The modified  $D_{oe}^{\text{th}}$  value can be written as

$$D_{oe}^{\text{th}} = \Delta + \lambda_2 + \delta . \quad (3)$$

In the practical calculations, the contribution from quadrupole pairing is included, though this term is not written explicitly in the above equation. However, as mentioned above, the contribution of the doubly-stretched quadrupole-pairing energies is very small (usually less than 30 keV in magnitude). In the right side of Eq.(3) the pairing gap,  $\Delta$ ,

is the dominant term. Obviously, due to the presence of the  $\delta$  term,  $D_{oe}^{\text{th}}$  is in general not equivalent to the pairing gap ( $\Delta + \lambda_2$ ) of even-even nuclei. The  $\Delta$  value is very sensitive to the change in the  $G$  value, while the  $\lambda_2$  and  $\delta$  values are not.

The presence of the negative  $\delta$  value implies that the pairing strength  $G$ , needs to increase when one aims at self consistent calculations of odd-even mass differences. By adjusting the pairing strength, one can reproduce the experimental  $D_{oe}$  value. However, in that case we found that each nucleus requires its separate determination of  $G$ . Apparently, the average gap method [11] does not have the proper particle-number and deformation dependence. Of course, other quantities contributing to the odd-even mass difference may be lacking in our model. One such effect is the coupling to phonons, which will influence the ground-state binding energy, depending on the softness of the nuclear shape. Also, displacements of the single-particle spectrum of the Woods-Saxon potential will affect the calculated  $D_{oe}$  values. To disentangle the different contributions, especially to optimize a method to determine the average pairing strength, is outside the scope of the present work.

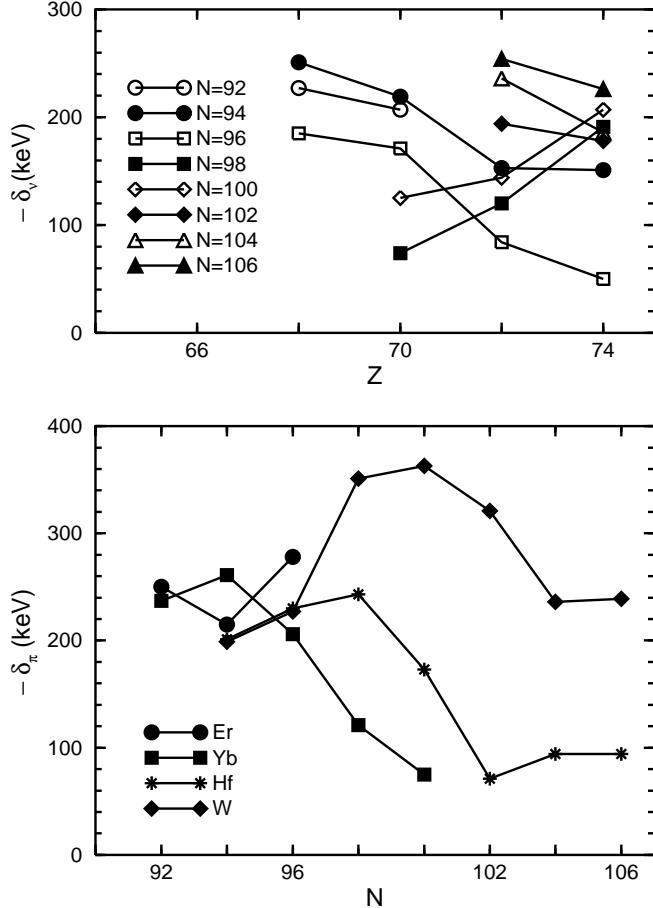


FIG. 1. Obtained shape and blocking effects ( $\delta = \delta_{\text{shape}} + \delta_{\text{block}}$ ) as a function of nucleon number. The upper panel is for neutrons ( $\nu$ ) and the lower panel for protons ( $\pi$ ). Note that the  $\delta$  values are negative.

In order to better reproduce the average of experimental  $D_{oe}$  values, we scale the pairing strength by  $G = FG^0$ , where  $G^0$  is the pairing strength obtained by the average gap method [11]. For reason of simplicity, we use a constant factor  $F$ , which we determine from individual  $F$  values that have been fitted to the corresponding  $D_{oe}^{\text{expt}}$  values in this mass region. We expect that using an average  $F$  value will reduce the fluctuations arising from the uncertainties of experimental masses and from possible discrepancies between theoretical and experimental single-particle levels. For the region of the studied nuclei, we obtain  $\tilde{F}_\nu = 1.08$  (neutrons) and  $\tilde{F}_\pi = 1.05$  (protons) using the experimental masses of Ref. [22]. This results in increases of the LN pairing gaps by about 25% for neutrons and 15% for protons.

To investigate the consistency of our method, we calculate the moments of inertia ( $J(\omega)$ ) of yrast rotational bands by means of the pairing-deformation self-consistent cranked shell model [23,24]. As mentioned at the beginning of the paper, the moment of inertia is a very sensitive probe of pairing correlations. It is not at all obvious, that a

pairing interaction that reproduces the odd even mass difference at the same time also can reproduce the moments of inertia. In Fig. 2, we compare experimentally deduced moments of inertia with the results of our calculations, done with the standard pairing strength  $G^0$ , and the adjusted  $G = \tilde{F}G^0$ . Clearly, the adjusted  $G$  values lead to improved descriptions of both moments of inertia and backbending frequencies. (No additional parameters are adjusted in the present calculations.)

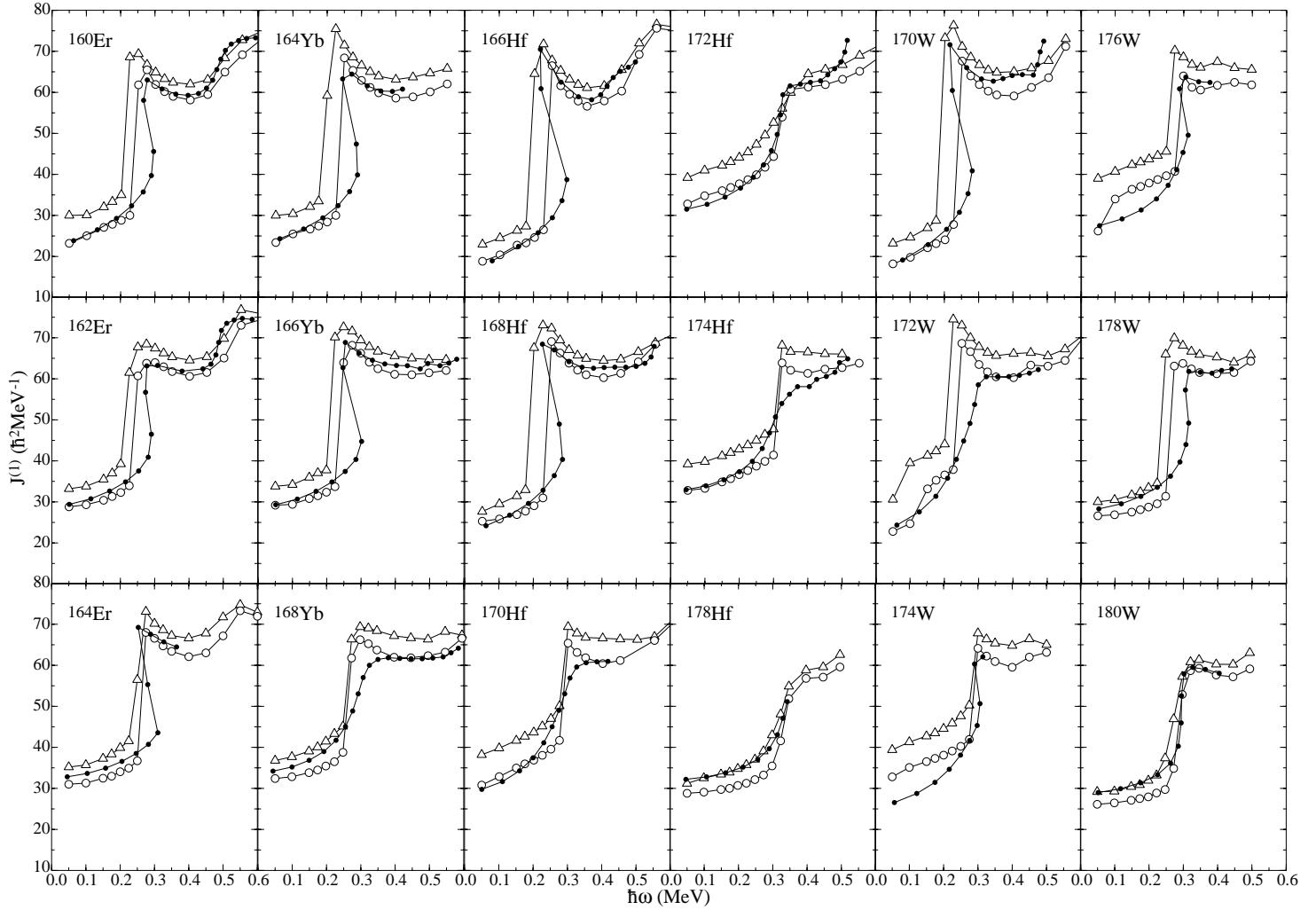


FIG. 2. Calculated and experimental moments of inertia. The open triangles and circles denote calculations with pairing strengths obtained by the average gap method ( $G^0$ ), and adjusted for average shape and blocking effects ( $G = \tilde{F}G^0$ ) respectively. The dots show the experimental values [25].

In this context, one needs to recall of the long standing problem of cranking calculations with monopole pairing, that do not at the same time describe both moments of inertia and band-crossing frequencies (see e.g. [8,9]). In order to reproduce moments of inertia, one in general needs to use a reduced pairing strength [9,7]. But on the other hand, an enhanced pairing field is required to reproduce band-crossing frequencies [8]. The presence of the time-odd component of the quadrupole pairing field [19,20], results in a stiffer nucleus, which allows an increase of the  $G$  value. Apparently, the doubly stretched quadrupole pairing interaction in combination with the Lipkin-Nogami

method enables a consistent description of both band crossing frequencies and moments of inertia.<sup>1</sup>

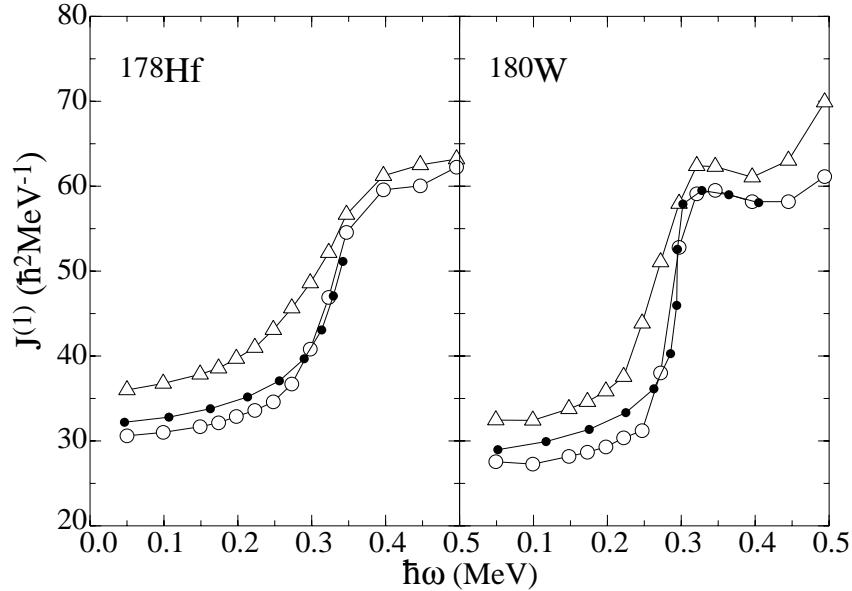


FIG. 3. Similar to Fig.2, but with the non-average  $G$  values. The open triangles are for the calculations with the  $G_0$  values which reproduce the  $D_{oe}^{\text{expt}}$  values with  $\Delta + \lambda_2$ . The open circles show the results with  $G/G_0 = 1.13$  (neutrons) and 1.05 (protons) in  $^{178}\text{Hf}$ , and correspondingly 1.10 and 1.09 in  $^{180}\text{W}$ , that reproduce the  $D_{oe}^{\text{expt}}$  values with  $\Delta + \lambda_2 + \delta$ .

For some heavy isotopes, however, using the average  $F$  values results in too small moments of inertia, e.g. in  $^{178}\text{Hf}$  and  $^{180}\text{W}$ . For these nuclei, the average  $F$  values give too large  $D_{oe}^{\text{th}}$  values. In fact, the  $\Delta + \lambda_2$  values obtained from  $G^0$  have already over-estimated the experimental odd-even mass differences for some heavy isotopes, e.g. by 166 keV (neutrons) and 190 keV (protons) in  $^{178}\text{Hf}$  and correspondingly 98 and 125 keV in  $^{180}\text{W}$ . In general, the average gap method gives too large  $\Delta + \lambda_2$  values for heavy isotopes and too small  $\Delta + \lambda_2$  values for light isotopes, indicating the problems of the  $A$ -dependence of the average gap method. Obviously, averaging the  $G$  adjusting factors does not change the  $A$ -dependence of the pairing gaps.

In order to check the influences from the possible discrepancy of the  $A$ -dependence of pairing gaps, we have also done the calculation with a pairing strength ( $G_0$ ) that reproduces the  $D_{oe}^{\text{expt}}$  value with  $\Delta + \lambda_2$  for each given nucleus. The  $G_0$  values are normally smaller than the average-gap-method  $G^0$  values for the heavy nuclei, e.g.  $^{178}\text{Hf}$  and  $^{180}\text{W}$ . Results show that the calculated moments of inertia with such  $G_0$  values are systematically larger than the corresponding experimental values. However, when instead the  $G_0$  values are adjusted by reproducing the  $D_{oe}^{\text{expt}}$  values with  $\Delta + \lambda_2 + \delta$  (i.e. including shape and blocking effects,  $D_{oe} = D_{oe}^{\text{expt}}$ ) a significantly improved description can be obtained, as shown in Fig.3 for the  $^{178}\text{Hf}$  and  $^{180}\text{W}$  examples. Here, we have obtained different  $F$  values (see Fig.3 caption) compared to the above average values, mainly because the different pairing strengths ( $G^0$  or  $G_0$ ) have been chosen as the reference of the  $G$  adjustment. The non-average  $F$  values are mostly in range of 1.05–1.10 for neutrons and 1.03–1.08 for protons. Clearly, the proper pairing strength for odd-even mass differences is also consistent with experimental moments of inertia. In addition, the increase of the pairing strength found in our work agrees with that needed to reproduce the excitation energies of high-seniority states [10].

Deformations, which can change with rotational frequency, are determined self-consistently by calculating the Total Routhian Surfaces (see e.g. [20,23,24]). With the determined deformations, the calculated intrinsic quadrupole moments ( $Q_0$  [10]) agree with corresponding experimental values [26]. The deformation changes due to the adjustments

<sup>1</sup>Other effects like the coupling to the vibrational phonons, that may affect the crossing frequencies are of course not taken into account

of the  $G$  values are very small ( $|\Delta\beta_2| < 0.003$  and  $|\Delta\beta_4| \leq 0.002$ ) for nuclei that are not soft. In  $^{172,176}\text{W}$ , some shifts in  $J(\omega)$  can be seen, which are due to the shifts of the  $\beta_2$  values with increasing rotational frequency. The PES calculations, as mentioned, for  $^{172-176}\text{W}$  are soft in  $\beta_2$ .

In summary, we have investigated the shape and blocking effects on odd-even mass differences for even-even rare-earth nuclei. These effects are shown to be in the range of 10–30% of the corresponding odd-even mass differences. The blocking effect, in principle, should belong to the category of pairing effects. Clearly, these effects should not be neglected in determining the pairing strengths. Indeed, when blocking and shape effects are taken into account, pairing strengths are increased by about 5–10% resulting in sizeable changes of the pair gaps. The adjusted strengths are consistent with what is needed to reproduce the excitation energies of multi-quasi particle configurations, and lead to an improved description of nuclear collective rotational motion, through calculating moments of inertia and backbending frequencies. The present work establishes a consistent relation between mass differences, moments of inertia and excitation energies of high seniority states.

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